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Metal–Insulator Transition in Randomly Interacting Systems

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We discuss a metal–insulator transition caused by random couplings of magnetic moments in itinerant systems. An analytic solution for the single particle Green function is derived from dynamical self consistency equations, the corresponding density of states is characterized by the opening of a gap. The scaling behavior of observables is analyzed in the framework of a scaling theory and different crossover lines are identified. A fluctuation expansion around the mean field solution accounts for both interaction and localization effects in a consistent manner and is argued to be relevant for the description of the recently discovered metal–insulator transition [1,2] in 2d electronic systems.

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Interaction driven metal–insulator transitions (MITs) as well as magnetism are among the most striking consequences of strong electronic correlations. For many years progress in the theoretical investigation of these phenomena was impeded by their manifestly nonperturbative nature, and only the introduction of powerful new methods like self-consistent dynamical mean field theories (DMFT) has initiated progress [3,4]. The modification of the disorder induced localization transition by interactions has been the subject of intensive studies [5], whereas the profound effects of random interactions on the band structure have attracted interest only recently [6,7] in the form of a hard gap causing a crossover from variable range hopping to activated behavior in the conductivity. In this letter we explore the phase diagram of metallic spin glasses in the vicinity of the quantum phase transition between a gapped insulating phase and a metallic phase (SG–MIT) with a density of states (DoS) at the Fermi level increasing continuously from zero as the magnetic interaction strength is reduced. Applications to the recently discovered MIT in 2d systems [1,2] and the spin glass phase in High T_c superconductors [8] are discussed.

While in clean systems the MIT so far can only be described with the help of numerical methods, the prevalence of disorder correlations in spin glasses makes it possible to find an analytic solution of dynamical mean field equations. A Hamiltonian with hopping elements out of the Gaussian orthogonal ensemble leads in infinite space dimensions to a set of equations equivalent to the local impurity self-consistent approximation (LISA) [4] as was already pointed out in [7]. For the typical magnetic interaction J much smaller than the kinetic energy the DoS is semicircular with a width $2E_0$ and the system is a metallic spin liquid, whereas for $E_0 = (32/3\pi)J$ a quantum transition from paramagnet to spin glass takes place [9–11]. A further decrease of E_0/J leads to a suppression of the DoS at the Fermi level ρ_F until at $E_{0c} = 2.59J$ a gap opens up. The dynamical selfconsistent theory treats both the disordered electron hopping and the spin–spin interaction in a consistent manner and is therefor a good starting point for a fluctuation expansion. From the appearance of replica symmetry breaking in the fluctuation theory it is conjectured that this transition is preceded by a Griffith phase in analogy with the ferromagnetic phase in the random field Ising model [12]. Thermal fluctuations affect the SG–MIT in a double way: they smear out the transition itself and they shift its location by reducing the magnetic correlations. These effects are described by crossover lines separating quantum critical, insulating and metallic behavior of DoS and transport coefficients. While in infinite space dimensions the SG–MIT has magnetic correlations at its origin, in finite space dimensions localization fluctuations become important and the transition has to be compared with the Anderson Mott MIT [5]. Both the existence of the order parameter DOS and the quartic critical theory [13] with a dangerously irrelevant variable suggest that the similarity persists in fluctuation theory. However, we expect that the detailed treatment of interaction effects in our mean field theory and the correct choice of the ground state will render the renormalization group (RG) theory of the SG–MIT free of instabilities present in the usual sigma model approach [14,15] to interacting disordered systems.

We study a single band model with the Hamiltonian

$$H = \sum_{i,j} t_{ij} c^{\dagger}_{i,\sigma} c_{j,\sigma} - \frac{1}{2}\sum_{i,j} J_{ij} S_i S_j \quad , \tag{1}$$

comprised of a kinetic part with real symmetric hopping matrix elements distributed according to a Gaussian probability measure with moments $< t_{ij} >= 0$ and $< (t_{ij})^2 >= M(i-j)$, and a random interaction between Ising spins with variance J^2 (SK model). It can be viewed as effective t–J model describing the interaction of spin fluctuations at randomly distributed impurity sites with strong Coulomb repulsion [16]. The disorder average is performed by means of the replica method, the replicated partition function is represented with the help of Grassmann integrals. The four fermion and four spin terms are decoupled with quaternionic ma-

trix fields $\underline{\underline{R}}^{ab}(x;\tau,\tau')$ and scalar fields $Q^{ab}(x;\tau,\tau')$. In infinite space dimensions dynamical saddle point equations become exact and the stationary values can be identified with the single particle Green function and the spin autocorrelation function, respectively. After further decoupling of the spin–spin interaction the fermions can be integrated out. For a replica symmetric and static approximation of the linear susceptibility and in the limit of zero temperature two of the three integrals over spin decoupling fields can be solved exactly by the method of steepest descent. One ends up with a spectral type self–consistency equation for the the thermal single particle Green function $G(\epsilon_l) = (4/iE_0^2)r_l$ with r_l denoting the saddle point value of the charge decoupling fields. The shortcomings of this calculation are remedied in the framework of a Landau Ginzburg theory for the SG–MIT, which allows to include the effects of finite temperature, inelastic interactions and replica symmetry breaking. The self–consistency equation for the Green function reads

$$r(\epsilon_l) = \frac{E_0^2}{4}(r_l+\epsilon_l) \quad \int_{-\infty}^{\infty} \frac{dz}{\sqrt{2\pi}} \frac{A(z)}{(r_l+\epsilon_l)^2+z^2} \qquad (2)$$

where the weight function is given by

$$A(z) = \frac{1}{\sqrt{q}}\theta[|z|-\chi_0|\phi'(z)|][1-\chi_0\phi''(z)]e^{-\frac{1}{2q}[|z|-\chi_0|\phi'(z)|]^2} \ . \qquad (3)$$

The Edwards Anderson order parameter $q = \lim_{t\to\infty} < S(t)S(0) >$ and the zero frequency component χ_0 of the local magnetic susceptibility have to be determined by extremizing the free energy, $\phi(z) = Tr\log[1+z^2/(r_l+\epsilon_l)^2]$ is a functional of the electron Green function, all energies and magnetic fields are measured in units of the average spin coupling J. The derivation of eqs.(2,3) will be presented elsewhere.

In order to gain insight into the behavior of the spectral type function $A(z)$ it is useful to calculate it non self-consistently for a semi-elliptic Green function and different values of the bandwidth E_0. Large values of E_0 yield a functional $\phi(z)$ with a maximum at $z=0$ and $A(z) = A_0 + O(z)$ for small z, consequently solutions of (2) are metallic. For $E_0 < 1.5$ however, ϕ develops a double peak structure and therefor the weight function A(z) is gapped around z=0. In this case the denominator in eq.(2) can be expanded in powers of $r_l+\epsilon_l$. Keeping only the leading frequency dependence and adding the dominant temperature correction the result reads

$$(\delta_0 - T\delta_1)r_l + \kappa(r_l)^3 = \epsilon_l \qquad (4)$$

where

$$\delta_0 = (\frac{4}{E_0^2 < \frac{1}{z^2} >} - 1), \qquad \kappa = \frac{< \frac{1}{z^4} >}{< \frac{1}{z^2} >}, \qquad (5)$$

and δ_1 is a positive constant. All expectation values are taken with respect to the weight function $A(z)$. For the special value of the bare band width $E_0 = 2/\sqrt{< 1/z^2 >}$ corresponding to $\delta_0 = 0$ one finds at zero temperature a solution of the form $r_l \sim sgn(\epsilon_l)\sqrt[3]{|\epsilon_l|}$ with a dynamical critical exponent $z = 3$. In order to locate the critical point we have performed a selfconsistent calculation of the Green function. To find an analytic expression for the functional Φ the self–energy is modeled by $r_l = \kappa(\frac{|\epsilon_l|}{\kappa})^{1/3}$ for $|\epsilon_l| < \Lambda$ with a cutoff Λ determined by the normalization condition for the DoS $1 = \int_{-\Lambda}^{\Lambda}\rho(\epsilon)$. A free propagator $G(\epsilon_l) = \frac{1}{i\epsilon_l}$ is used for energies larger than the cutoff Λ. The functional Φ is in this approximation given by

$$\Phi(z) = \frac{1}{2\pi}\left[2\Lambda\ln\frac{1+\frac{z^2\Lambda^{2/3}}{\kappa^{4/3}}}{1+\frac{z^2}{\Lambda^2}} + 2\pi|z| - 4z\arctan\frac{\Lambda}{z} \right. \qquad (6)$$
$$\left. +\frac{4}{3}z^2\left(\frac{3\Lambda^{1/3}}{\kappa^{4/3}} - \frac{3z}{\kappa^2}\arctan\frac{\kappa^{2/3}\Lambda^{1/3}}{z}\right)\right].$$

Using this functional we have solved numerically the system of coupled selfconsistency equations for critical band width, local susceptibility, and spin glass order parameter, and found the result $E_{0c} = 2.53J$, $\chi_{0c} = 0.79/J$, and $q_c = 0.66$. We have verified that a solution $\sim \sqrt{\epsilon_l}$ corresponding to a parabolic gap in A(z) does not satisfy eq(2,3).

To discuss various crossover scenarios one needs the full solution for the single particle Green function, though. It is given by

$$G(\epsilon_l) = \frac{-4i}{E_0^2}\left\{\frac{-\delta}{3\kappa^{2/3}[\frac{\epsilon_l}{2}+\sqrt{\frac{\delta^3}{27\kappa}+(\frac{\epsilon_l}{2})^2}]^{1/3}} \right.$$
$$\left. +\kappa^{-1/3}[\frac{\epsilon_l}{2}+\sqrt{\frac{\delta^3}{27\kappa}+(\frac{\epsilon_l}{2})^2}]^{1/3}\right\} \ . \qquad (7)$$

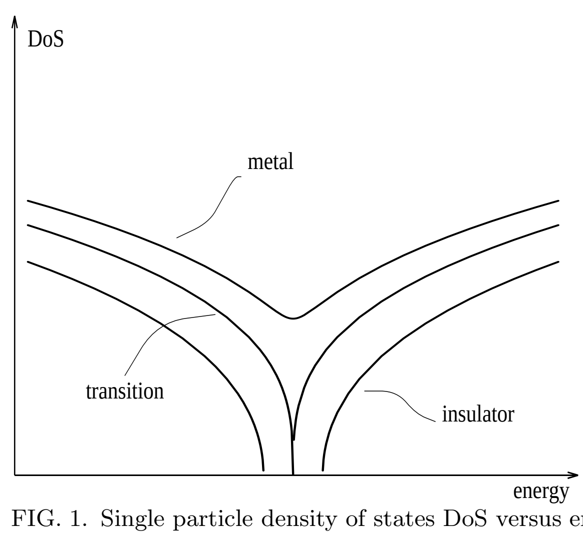

FIG. 1. Single particle density of states DoS versus energy for different values of the electron hopping strength corresponding to metallic, critical and insulating behavior.

Here $\delta = \delta_0 - T\delta_1$ plays role of a mass squared which separates the disordered (insulating) phase with positive δ and vanishing ρ_F from the ordered (metallic) phase. The dependence of the DoS on the bare bandwidth E_0 is displayed in fig.(1). The temperature dependence of δ describes the effects originating in the reduction of magnetic correlations by thermal fluctuations. The DoS at the Fermi level depends on temperature via $\rho_F = \frac{4}{\pi E_0^2}\sqrt{\frac{-\delta}{\kappa}}$. For low T the constant term δ_0 dominates and the DoS is approximately constant, whereas for $T \gg \frac{-\delta_0}{\delta_1}$ thermal fluctuations take over and the system behaves as if it were at its quantum critical point. Hence for all observables dominated by the critical DoS, the quantum critical (QC) region is delimited by the lines $T = \frac{|\delta_0|}{\delta_1}$, see fig.(2).

Given the fact that in the replica symmetric solution of the SK–model (as well as in simulations of finite dimensional spin glasses) the distribution of local fields $P(h_{loc})$ is nonzero for $h_{loc} = 0$ it is questionable whether the frozen in magnetic moments in a spin glass can cause a gap in the single particle DoS and drive the system insulating. The investigation of generalized Thouless–Anderson–Palmer (TAP) equations [7,17] suggests that a spin at site i lowers its energy by polarizing its neighborhood. The resulting self energy $E_g = [\sum_j \chi_{jj}(J_{ij})^2]_{av}$ favors the single occupation of sites and thus insulating behavior. The influence of replica symmetry breaking and finite range interactions on the magnetic self energy are discussed in [7,18,19].

For finite dimensional systems the DC conductivity is calculated to leading order in a $1/N$–expansion [20] from the density–density response function $D(q,\omega_n)$ utilizing the Kubo relation

$$\sigma_{DC} = -e^2 \lim_{\omega\to 0} \omega \lim_{q\to 0} \frac{\partial}{\partial q^2} Im D^R(q,\omega) \quad . \tag{8}$$

The result $\sigma_{DC} = e^2\rho_F D$ with the charge diffusion constant $D = 2\pi b_m \rho_F$ (b_M being the second Fourier coefficient of the hopping correlation function M(q)) exhibits a linear dependence on T in the QC region since there the DoS is suppressed like $\sqrt{T}$.

The results of the last paragraphs can be collected in the unifying framework of a scaling theory. In the finite temperature formalism the DoS $\rho(\epsilon_l) = -\frac{\partial \beta F}{\partial \epsilon_l}$ is the derivative of the free energy with respect to an external frequency ϵ_l. This external frequency is analogous to an external field in the context of a magnetic phase transition, a nonvanishing ρ_F breaks the symmetry between advanced and retarded energies. The transition is sharp for zero external field, whereas in the general case the DoS obeys the scaling relation $\rho \sim |\delta|^\beta \mathcal{R}_\pm(\frac{\epsilon}{|\delta|^{z\beta}})$. The limiting behavior of the scaling function is $\lim_{x\to\infty}\mathcal{R}_\pm(x) = x^{1/z}$ and $\lim_{x\to 0}\mathcal{R}(x) \sim \theta(\mp 1)$. The two relevant scaling fields T and $E_0 - E_{0c}$ are related by a crossover exponent $\phi = 1$ and hence can be combined in a single variable δ. From the denominator $\omega_n + Dq^2$ of the diffusive two particle propagator one determines the scaling behavior of the diffusion constant as

$$D \sim \delta^{\nu(z-2)} \quad , \tag{9}$$

and inferring the violation of hyper-scaling derived from the RG analysis we finally obtain

$$\sigma_{DC} \sim \delta^{\nu(d-\theta_t-2)} \quad . \tag{10}$$

So far all results have been obtained in the framework of a replica symmetric and spin static dynamical mean field calculation. In the following we will argue that the physics of a finite dimensional system with replica symmetry breaking and inelastic many–particle interactions is correctly described by a dynamical Landau–Ginzburg theory.

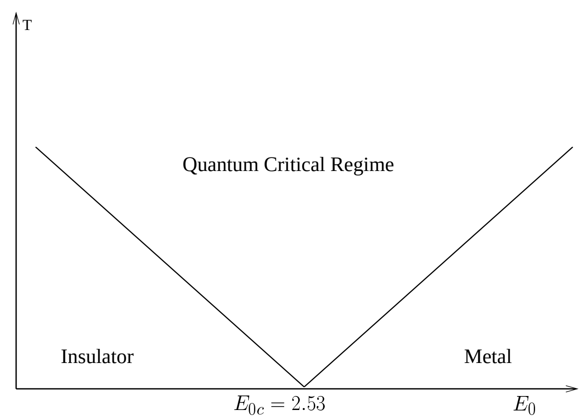

FIG. 2. Phase diagram in the vicinity of the SG–MIT at a bare bandwidth $E_0 = 2.53J$. The transition lines separate the quantum critical region with a $T^{1/2}$–dependence of the DoS from the insulating regime with a gap at lower E_0 and from the metallic region.

In order to calculate critical properties of the *finite dimensional* SG–MIT we have expanded the free energy in fluctuations about the dynamic mean field solution. The fluctuation fields are hermitian $4n \times 4n$ matrices which depend on two time and one space variable. They obey charge conjugation symmetry in the form $\underline{\underline{C}}\,\underline{\underline{R}}^T\underline{\underline{C}}^T = \underline{\underline{R}}^\dagger$ with the charge conjugation matrix $\underline{\underline{C}} = i\sigma_2 \otimes \sigma_0$. We obtained for the quantum action governing the critical theory after a suitable rescaling of space and time variables

$$\begin{aligned}
\mathcal{A} = \frac{1}{t}\int d^d x \{ & T^2 \sum_{\epsilon_l,\epsilon_k} R^{ab}_{\alpha\beta}(x;\epsilon_k,\epsilon_l)[(-\nabla^2 + \epsilon_k^{2/3} + \epsilon_l^{2/3} \\
& + \epsilon_k^{1/3}\epsilon_l^{1/3} + 1)\delta_{\alpha\delta}\delta_{\beta\gamma} - \gamma^z_{\alpha\delta}\gamma^z_{\beta,\gamma}] R^{ba}_{\gamma\delta}(x;\epsilon_l,\epsilon_k)\} \\
& + \frac{T^2}{t}\sum_{\epsilon_l,\epsilon_k} R^{aa}_{\alpha\beta}(x;\epsilon_k,\epsilon_k)\gamma^z_{\beta\alpha} r^{ab}\gamma^z_{\gamma\delta} R^{bb}_{\delta\gamma}(x;\epsilon_l,\epsilon_l) \\
& + uT^3 \sum_{\epsilon_k,\epsilon_l,\epsilon_m} R^{aa}_{\alpha\beta}(x;\epsilon_k,\epsilon_l)\gamma^z_{\beta\alpha}\gamma^z_{\gamma\delta} R^{aa}_{\delta\gamma}(x;\epsilon_m,\epsilon_k - \epsilon_l + \epsilon_m)
\end{aligned}$$

$$+\frac{\kappa_1}{4!}Tr[(\underline{\underline{R}}\underline{\underline{\gamma^z}})^4] + \frac{\kappa_2}{4!}Tr[(\underline{\underline{R}}\underline{\underline{\gamma^z}})^2]^2\}. \tag{11}$$

Here $\gamma^z = \sigma_0 \otimes \sigma^z$ is a spin matrix and r^{ab} depends on the Parisi solution of the spin glass problem. The $4n^2$ critical modes satisfy $\underline{\underline{R}}\underline{\underline{\gamma^z}} = \underline{\underline{\gamma_z}}\underline{\underline{R}}$. Note that the quantum interaction u has no influence on the mean–field solution as for a spin glass there is no net magnetization. The spin glass order parameter q^{ab} modifies the random field term and describes the influence of frozen magnetic moments. The dangerously irrelevant variable t is already introduced at tree level to account for the shift of the upper critical dimension caused by disorder correlations. Due to the presence of replica symmetry breaking the value of its exponent θ_t will be different from 2 already in a two loop RG calculation. From the presence of replica symmetry breaking the appearance of a glassy phase preceding the SG–MIT can be conjectured in analogy to [12].

In a tree level RG–analysis the quantum mechanical many–body interaction u is found to be irrelevant with scaling exponent $-\theta_u = -1$ in the vicinity of the upper critical dimension $d_c^{(u)} = 6$. Actually u is dangerously irrelevant and changes the crossover line between metallic and quantum critical region from the naively expected $T \sim \delta^{z\nu}$ to $T \sim \delta^{(z\nu)/(1+\theta_u\nu)}$. As long as the quantum dynamics are irrelevant the lower critical dimension $d_c^{(l)}$ of the model is expected to be equal to two. However, if the interaction term becomes relevant in low spatial dimensions as it happens in the Finkel'stein theory of interacting electrons, it will shift $d_c^{(l)}$ below two. This effect of a reduced lower critical dimension is well known in models with relevant quantum dynamics. Recently a MIT has been observed in high–mobility metal–oxide–semiconductor field–effect transistors (MOSFETs) [1,2] and a variety of other 2d systems. These experiments challenged the widely held belief that two is the lower critical dimension for MIT's in all types of disordered systems. The RG theory of the MIT in interacting systems [14,15] indeed admits the possibility of a metallic phase but is hampered by the occurrence of a magnetic instability in the triplet channel. A transition to a ferromagnetic state seems unlikely as the 2d metallic phase is quenched by a parallel magnetic field [22]. Since randomness is relevant in these materials it is reasonable to expect spin glass freezing of magnetic moments. The divergence of the triplet amplitude in the RG theory [14,15] occurs at a finite length scale, therefor the frozen moments are most likely not single spins but ferromagnetically ordered clusters. These ordered clusters may form in regions with strong disorder, interact via a RKKY type interaction mediated by conduction electrons, and form a Stoner glass [16]. The freezing of magnetic moments as represented by the random field term in eq.(11) reduces the magnetic susceptibility and is expected to control the runaway flow in a RG analysis. The validity of these ideas can be tested by performing magnetic measurements and looking for irreversibilities indicative of random freezing of magnetic moments.

In perovskite materials with narrow bands and a pronounced spin glass phase like LaSrCuO on the other hand there should be a possibility to observe the interaction driven SG–MIT by lowering the temperature below the spin glass freezing temperature.

In summary, we derived dynamical selfconsistency equations describing itinerant systems with random magnetic couplings. The analytic solution displays a metal–insulator transition due to magnetic correlations. The mean field theory served as a starting point for the derivation of a fluctuation theory describing the combination of localization and interaction fluctuations. The effects of randomly frozen magnetic moments are described by a random field term, and from the appearance of replica symmetry breaking in this term the presence of a glassy phase preceding the MIT was conjectured.

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